Formal Proof of SCHUR Conjugate Function* **

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Abstract. The main goal of our work is to formally prove the correctness of the key commands of the SCHUR software, an interactive program for calculating with characters of Lie groups and symmetric functions. The core of the computations relies on enumeration and manipulation of combinatorial structures. As a first "proof of concept", we present a formal proof of the conjugate function, written in C. This function computes the conjugate of an integer partition. To formally prove this program, we use the Frama-C software. It allows us to annotate C functions and to generate proof obligations, which are proved using several automated theorem provers. In this paper, we also draw on methodology, discussing on how to formally prove this kind of program.

1 Introduction

SCHUR [1] is an interactive software for calculating properties of Lie groups and symmetric functions [2]. It is used in research by combinatorists, physicists, theoretical chemists [3] as well as for educational purpose as a learning tool for students in algebraic combinatorics. One of its main uses is to state conjectures on combinatorial objects. For such use, it is important to have some confidence in the results produced by SCHUR.

Until now, the method used to get some confidence in the results has mostly been based on just one example for each command.

The computation of other examples is complex due to the well known combinatorial explosion, especially when using algorithms associated to the symmetric group, see section 2.1. Unfortunately, the combinatorial explosion as well as computing time forbid test generation or verification techniques (model checking). Therefore, in this paper, we focus on formal proof of the existing program.

With the aim of verifying the whole software, we start with proving the correctness of its fundamentals bricks. The main combinatorial object used in SCHUR is integer partition. The first non-trivial operation on integer partitions is the conjugate. Moreover, conjugate function is necessary for more than half of the 240 interactive commands of SCHUR. From this point of view, we can say that conjugate is a critical function of SCHUR.

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The very first work consists in isolating (see 4.3) the code of this function from the program. Next, we chose to use the most popular tool of program proof community's Frama-C [4] successor of Caduceus. Frama-C is a plug-in system. In order to prove programs, we used Jessie [5], the deductive verification plug-in of C programs annotated with ACSL [6]. The generated verification conditions can be submitted to external automatic provers, and for more complex situations, to interactive theorem provers as well (see section 2.2).

After a short presentation of software tools and theoretical concepts, we will present the formal proof of a program. Finally, after discussing difficulties and mistakes encountered along the way, we will propose a methodology to prove such a software, and finally discuss future work.

2 Presentation of the Software Used

2.1 The SCHUR Software

SCHUR is an interactive software for calculating properties of Lie groups and symmetric functions. A Symmetric Function is a function which is symmetric, or invariant, under any permutation of its variables. For example $f(x_1, x_2, x_3) = x_1 + x_2 + x_3$ is a symmetric function.

SCHUR has originally written by Prof. Brian G. Wybourne in Pascal language. Then it was translated into C by an automatic program making it quite difficult to read. There are almost no comments in the code, the code is more than 50,000 lines long with many global variables. Local variables have names such as W52 and so on.

After the death of Prof. Wybourne in November 2003, some people felt that his program should be maintained, and if possible enhanced, with a view to making it freely available to the mathematics and physics research community.

Nowadays, it is open source under the GPL license and includes more than 240 commands. The code still includes very few comments. Some mistakes have been corrected but some interactive commands are so intricate that it is difficult to have more than a few examples to check them against and most people do not even know if the result is correct or not.

This is why we started to work on this code. Firstly some of the commands in SCHUR are very well implemented (for example, plethysm is computed faster by SCHUR than by many other combinatorial toolboxes). Formally proving some key functions inside would also be a major advance for its research community.

2.2 The Frama-C Software

Frama-C [4] is an open source extensible platform dedicated to source code analysis of C software. It is co-developed by two French public institutions: CEA-LIST (Software Reliability Laboratory) and INRIA-Saclay (ProVal project).

Frama-C is a plug-in system. In order to prove programs, we use Jessie [5], the deductive verification plug-in of C programs annotated with ACSL [6]. It

uses internally the languages and tools of the Why platform [7]. The Jessie plug-in uses Hoare-style [8] weakest precondition computations to formally prove ACSL properties. The generated verification conditions (VC) can be submitted to external automatic provers such as Simplify [9], Alt-Ergo [10], Z3 [11], CVC3 [12].

These automatic provers belong to SMT (Satisfiability Modulo Theories) solvers. The SMT problem is a decision problem for logical formulas with respect to combinations of background theories expressed in classical first-order logic with equality. First-order logic is undecidable. Due to this high computational difficulty, it is not possible to build a procedure that can solve arbitrary SMT problems. Therefore, most procedures focus on the more realistic goal of efficiently solving problems that occur in practice.

For more complex situations, interactive theorem provers can be used to establish the validity of VCs, like Coq [13], PVS [14], Isabelle/HOL [15], etc. For our purpose, we used Coq (see section 4.2) since it is the one best known to the authors.

3 The Conjugate Function

In this section, the basics of algebraic combinatorics are given so that the reader can understand what is actually proved. Interestingly in this field, though the interpretation of what is actually computed can be of a very abstract algebraic level, the computation itself boils down most of the time to possibly intricate but rather elementary manipulations.

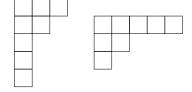
3.1 Combinatorial and Algebraic Background: Integer Partitions

A partition of a positive integer n is a way of writing n as a sum of a non-increasing sequence of integers. For example $\lambda = (4, 2, 2, 1)$ and $\mu = (2, 1)$ are partitions of n = 9 and n' = 3 respectively. We write $|\lambda| = n$ and $|\mu| = n'$ [16].

The **Ferrers diagram** F^{λ} associated to a partition $\lambda = (\lambda_1, \lambda_2, ..., \lambda_p)$ consists of $|\lambda| = n$ boxes, arranged in $l(\lambda) = p$ left-justified rows of lengths $\lambda_1, \lambda_2, ..., \lambda_p$. Rows in F^{λ} are oriented downwards (or upwards for some authors). F^{λ} is called the shape of λ .

Definition 1. The conjugate of an integer partition is the partition associated to the diagonal symmetric of its shape.

For example, for $\lambda = (3, 2, 1, 1, 1)$, here is the Ferrers diagram F^{λ} and the Ferrers diagram of the conjugate partition:



So the conjugate partition of (3, 2, 1, 1, 1) is (5, 2, 1).

A semi-standard Young tableau of shape λ is a numbering of the boxes of F^{λ} with entries from $\{1, 2, ..., n\}$, weakly increasing across rows and strictly increasing down columns. A tableau is **standard** if and only if each entry appears only once. Here is an example of shape (4, 2, 2, 1) tableau:

1	2	2	5
2	4		
3	6		
5			

A symmetric function of a set of variables $\{x_1, x_2, ...\}$ is a function $f(x_1, x_2, ...)$ of those variables which is invariant under any permutation of those variables (that is for example $f(x_1, x_2, ...) = f(x_2, x_1, ...)$). This definition is usually restricted to polynomial functions. The most important linear basis of symmetric function's algebra is called the **Schur functions** and they are combinatorially defined as follows: for a given semi-standard Young tableau T of shape λ , write \mathbf{x}^T the product of the x_i for all i appearing in the tableau. Then

$$s_{\lambda}(\mathbf{x}) = \sum_{T \in \text{Tab}(\lambda)} \mathbf{x}^{T}.$$
 (1)

where $\text{Tab}(\lambda)$ is the set of all tableaux of shape λ . We will note $s_{\lambda}(\mathbf{x})$, s_{λ} . For example, consider the tableaux of shape (2,1) using just three variables x_1, x_2, x_3 :

1	1	1	1	2	2	1	2	1	3	1	2	1	3	2	3
2		3		3		3		2		2		3		3	

The associated Schur function is therefore:

$$s_{(21)}(x_1, x_2, x_3) = x_1^2 x_2 + x_1^2 x_3 + x_2^2 x_3 + 2x_1 x_2 x_3 + x_1 x_2^2 + x_1 x_3^2 + x_2 x_3^2$$
 (2)

thus:

$$s_{(21)} = s_{(21)}(x_1, x_2, x_3) + s_{(21)}(x_1, x_2, x_3, x_4) + \dots$$

Note that, with this combinatorial definition, the symmetry of $s_{(21)}(x_1, x_2, x_3)$ is not exactly obvious.

We need to recall some well-known results in symmetric function theory: though Schur functions have historically been defined by Jacobi [17], they were named in the honor of Schur who discovered their crucial role in the representation theory of the symmetric group and the general linear group. Namely, after the discovery by Frobenius that the irreducible representation of the symmetric groups are indexed by integer partitions, Schur showed that those functions can be interpreted as characters of those irreducible representation, and by Schur-Weyl duality characters of Lie groups and Lie algebras. Notably we obtain the representation of the general linear groups (GL_n) and unitary groups (U_n) [18] from the symmetric group representations. In this setting, the conjugate of the

partition essentially encodes the tensor product of a representation by the sign representation.

Further work by Schur-Littlewood involve infinite sum of Schur functions associated to partitions [19], whose conjugates have a particular form. In particular, these series are used to obtain symplectic (Sp_{2n}) and orthogonal character groups (O_n) (symmetric and orthogonal Schur functions) from standard Schur functions [20].

One particularly important and difficult computational problem here is plethysm (see SCHUR reference manual [1] and [2]). It is the analogue in symmetric functions of the substitution of polynomial inside another polynomial $f(x) \mapsto f(g(x))$. It is called plethysm because by some combinatorial explosion, it involves very quickly a lot (a plethora) of terms, making it something very difficult to compute efficiently. For example, $s_{(21)}(s_{(21)})$, the first example with non trivial partitions in the input is already very hard to compute by hand. First we can regard $s_{(21)}$ as a function in as many monomial as in (2):

$$s_{(21)}(s_{(21)})(x_1,x_2,x_3) = s_{(21)}(x_1^2x_2,x_1^2x_3,x_2^2x_3,x_1x_2x_3,x_1x_2x_3,x_1x_2^2,x_1x_3^2,x_2x_3^2)$$
 it can be shown that the following holds:

$$\begin{split} s_{(21)}(s_{(21)}) &= s_{(22221)} + s_{(321111)} + 2s_{(32211)} + s_{(3222)} + s_{(33111)} + \\ &3s_{(3321)} + 2s_{(42111)} + 3s_{(4221)} + 3s_{(4311)} + 3s_{(432)} + \\ &s_{(441)} + s_{(51111)} + 2s_{(5211)} + s_{(522)} + 2s_{(531)} + s_{(54)} + s_{(621)} \end{split}$$

3.2 Computation in Algebraic Combinatorics

Basically, the architecture of a software for computing in algebraic combinatorics is composed of two parts:

- a computer algebra kernel dealing with the bookkeeping of expressions and linear combinations (parsing, printing, collecting, Gaussian and Groebner elimination algorithm...);
- a very large bunch of small combinatorial functions which enumerate and manipulate the combinatorial data structures.

In algebraic combinatorics software, for each basic combinatorial structure such as permutations or partitions, there are typically 50-200 different functions. Conjugating a partition is a very good example of what those many functions do, that is surgery on lists of integers or lists of lists of integers or more advanced recursive structures like trees... In a basic computation, most of the time is spent mapping or iterating those functions on some sets of objects. But due to combinatorial explosion those sets can be very large so these functions must be very well optimized.

3.3 Properties

The definition of conjugate (diagonal symmetric of its partition shape) is easy to understand but may conduct to naive implementations that may be inefficient.

Let us suppose that we represent an integer partition by an integer array starting from 1. For example $\lambda = (3, 2, 1, 1, 1)$ gives t[1] = 3, t[2] = 2,... $t[l(\lambda)] = 1$. Recall that t[i] is non-increasing, that is $t[i+1] \leq t[i]$.

One way to compute the conjugate is to count boxes: in our previous example the first column of λ had 4 boxes, the second had 3 etc. Therefore, to compute the number of boxes in a column j we need to know how many lines are longer than j. As a consequence, if t_c is the array representing the conjugate, the following formula gives the value of the entries of the conjugate:

$$t_c[j] = |\{i \mid 1 \le i \le l(\lambda) \land t[i] \ge j\}|$$
.

Note that $t_c[j] = 0$ if j > t[1], so the previous expression must be computed only from j = 1 to j = t[1]. This last property will be one of our predicates used to check the correctness of loop invariants.

3.4 SCHUR Implementation

Here follows the code of the conjugate function extracted from the SCHUR software. We expanded type definitions (C "structs" and "typedefs") from the original code just to simplify the work of Frama-C and to make this part of code independent from the rest of the SCHUR software (getting rid of global variables and so on).

```
#define MAX 100

void conjgte (int A[MAX], int B[MAX]) {
  int i, partc = 1, edge = 0;

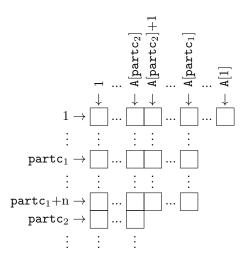
while (A[partc] != 0) {
   edge = A[partc];
   do
        partc = partc + 1;
   while (A[partc] == edge);
   for (i = A[partc] + 1; i <= edge; i++)
        B[i] = partc - 1;
}
</pre>
```

Note that this implementation is not naive (and not so easy to understand) but its time complexity is optimal (linear in the length of the partition).

The algorithm is based on looking for the set of descents of the partition⁵. The do—while loop follows a "flat" portion of the partition (t[i] = t[i-1]) until a descent is found. Next the for—loop assigns the values of the B array according to the flat portion. The following figure clarifies this: we have denoted $partc_1$ the value of partc at the entrance of while loop. $partc_2$ is the value of partc after

⁵ A descent is such that t[i] < t[i-1]

the do-while loop. For clarity's sake we supposed $A[partc_2]+1$ to be different from $A[partc_1]$. If we count boxes column by column to construct array B, it is clear that $B[i]=partc_2-1$ for all $A[partc_2]+1 \le i \le A[partc_1]=edge$.



4 The Formal Proof of the Conjugate Function

4.1 Annotations

In the following paragraphs we present the annotations added to the code. Note that this is the only additions made to it. First we have to specify the model of integers we want to deal with:

#pragma JessieIntegerModel(strict)

This means that int types are modeled by integers with appropriate bounds, and for each arithmetic operation, it is mandatory to show that no overflow occurs.

Next, we have to express in first-order logic what an integer partition (stored in an array) is:

```
#define MAX 100
/*@ predicate is_partition{L}(int t[]) =
      (\forall integer i; 1 <= i < MAX ==> 0 <= t[i] < (MAX-1)) &&
      (\forall integer i,j; 1 <= i <=j < MAX ==> t[j] <= t[i]) &&
      t[MAX-1] ==0;
      */</pre>
```

Note that annotations are coded in the C comments, starting with a @. The $\{L\}$ term is the context (pre, post, etc.), we won't detail it here, see [5,6] for details.

The data structure (array of integers) comes from the way the SCHUR software represents integer partitions. 0 is used as a mark of end of array, just like character strings in C. The MAX value comes from the original source code as well. The first line of the predicate <code>is_partition</code> expresses that we are able to compute the conjugate (if at least one element is greater than or equal to MAX-1, the conjugate will no be able to be stored in an array of size MAX-1 with the last element fixed to 0). From the source code it is expressed by an external simple test on t[1], but expressing it like that simplifies automatic provers job. The second line of the predicate defines the non-increasing order.

The following predicate is needed to express how we count blocs to compute the conjugate. It may be read as z equals the number of elements of partition t, whose indexes are included in $\{1, ..., j-1\}$ and whose values are greater than or equal to k. It is theoretically possible to express it as an axiomatic theory, a kind of function, but automatic provers we use make a better use of predicates. Note that we need to explicit the z=0 case, in order to be able to prove the global post-condition is_conjugate(A,B).

```
/*@ predicate countIfSup{L}(int t[],integer j,integer k,integer z)=
    is_partition{L}(t) &&
    1<= j <= MAX &&
    1<= k < MAX &&
    ((1<=z<j && \forall integer i ; 1<=i<=z ==> t[i]>= k)
    || (z==0 && \forall integer i ; 1<=i<j ==> t[i]<k)) ;
*/</pre>
```

Here is what we want to obtain at the end of the computation, t2 is a conjugate of t1 if the following holds:

```
/*@ predicate is_conjugate{L}(int t1[], int t2[]) =
    \forall integer k ; 1<=k<MAX ==> countIfSup(t1,MAX,k,t2[k]);
    */
```

Finally, here is the function. First we have to give precise requirements on the inputs. For example, (\valid(A+ (1..(MAX-1))) means that memory has been allocated so array indexes from 1 to MAX-1 are allowed). From the original code, the B array is supposed to be initialized with zeros before calling the function. This is translated into a requires directive. Next, we specify which memory elements are modified by the function (assigns). This is used for safety proofs. In the end, the output is correct if the post-condition (ensures) is met.

```
/*@ requires \valid(A+ (1..(MAX-1)));
  requires \valid(B+ (1..(MAX-1)));
  requires is_partition(A);
  requires \forall integer k; 1<=k<MAX ==> B[k]== 0;
  assigns B[1..A[1]];
  ensures is_conjugate(A,B);
  */
```

```
void conjgte (int A[MAX], int B[MAX])
{
  int i, partc=1, edge = 0;
```

Now we have to define the loop variant and invariant for each loop (to prove properties). The "loop variant" must decrease, while remaining non negative, to be able to prove termination. We also use a "ghost variable" to store the state of a variable before any modification.

```
/*@ loop variant MAX-partc;
    loop invariant 1<=partc<MAX;</pre>
   loop assigns B[1..A[1]];
    loop invariant \forall integer k;
       A[partc]+1 <=k <= A[1] ==> countIfSup(A,MAX,k,B[k]);
while (A[partc] != 0) {
   edge = A[partc];
   /*@ ghost int old_partc = partc; */
  /*@ loop variant MAX-partc;
      loop invariant old_partc<=partc ;</pre>
      loop invariant \forall integer k;
          old_partc<= k <= partc ==> A[k]==edge;
      loop invariant partc<MAX-1;</pre>
   */
   do
       partc = partc + 1;
   while (A[partc] == edge);
```

We also use the assert directive to have a verification point of a property that may help automatic provers for the next properties or global ones.

```
/*@ assert countIfSup(A,partc,edge,partc-1);*/

/*@ loop variant edge-i;
    loop invariant i >= A[partc]+1 && edge+1>=i ;
    loop invariant \forall integer k;
        A[partc]+1 <=k <i ==> countIfSup(A,MAX,k,B[k]);
    loop assigns B[ (A[partc]+1)..edge];
    */
    for (i = A[partc] + 1; i <= edge; i++)
        B[i] = partc - 1;
}</pre>
```

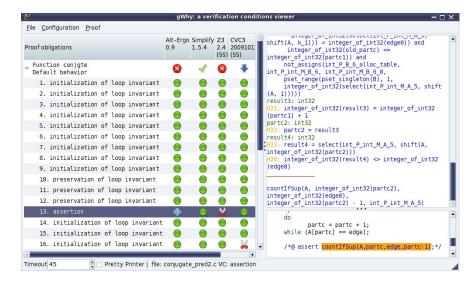


Fig. 1. Graphical Interface: default behavior

4.2 Proofs

The figures 1 to 3 are snapshots of gWhy (Frama-c graphical interface when using plugin Jessie). We applied this tool on the previous annotated code.

The Verification Conditions (VC, also called proof obligations) that have to be proved one by one (line by line) appear to the left of each of the following snapshots. In the upper right part of the window, we can check at a glance what hypotheses are known and what is to be proved at the bottom of it (under the line). No circularity paradox is possible here, since the proof of a VC can only rely on other VC higher in the control-flow graph of the function.

In the lower right part of the window, the corresponding part of the annotation is highlighted in the source code with some lines before and after it.

We will now focus on the VC part, to the left. We can see (green) dots meaning that this property has been proved by this prover. There is also (blue) rhombus with a question mark inside (see assertion 13), indicating that this prover will not be able to to prove this property. Actually, this does not mean that this VC is wrong, remember that these provers use heuristics. Sometimes, you may see scissors meaning that the maximum execution time has been reached without proving the VC. Again, this does not mean that the corresponding VC is wrong. Finally, at the top of a column a (green) check or (red, with a white cross inside) point is shown. The first one means that all properties have been proved by that prover. In fig.1, The (blue) arrow at the top of the CVC3 column means that it is still computing some unshown VC (greater than number 16).

The last figure is the final part. The provers have worked on the safety of the code, that is to say, integer bounds (overflow problems), pointer referencing and termination.

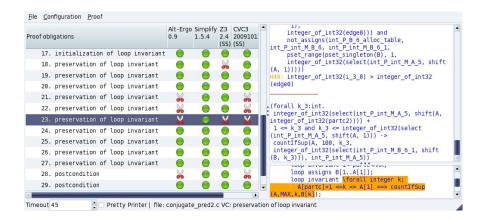


Fig. 2. Graphical Interface continued

As seen in section 4.1, the B array has to be initialized with zeros before calling the function. This requirement has been enlightened thanks to the annotations and tools, in particular because without the line requires \footnote{Trigon} integer k;1<=k<MAX ==> B[k]==0, the postcondition which states that B is a conjugate of A cannot be proved.

We have also used Coq proof assistant. However, it not being essential to our present point, we chose to live aside the detail of this procedure (see section 4.3).

4.3 Problems, Mistakes

As usual when using formal proof tools, there are several ways to formalize or to annotate programs. Choices made during at this stage are very important for future proofs. For example, declaring a function as an axiomatic theory or as a predicate will suppose corresponding proofs to be different. We can make a similar remark with data-types used in programs.

For these reasons, using "good" annotations which allows automatic provers to prove verification conditions (VC) successfully is a clever way to go about it.

When we deal with 40,000 lines of undocumented code, another critical part of the work consists in "correctly" isolating the piece of code that we want to prove. The code can use global variables, initializations made by other functions, or use intricate data-types and so on.

In the following paragraphs, these problems and associated mistakes are discussed.

Isolating a Part of Program. Generally speaking, the analyzed function must be free of external calls. More precisely if a function is called from it, it has to be incorporated in the code (like macro expansion) or, at least, independently proved.

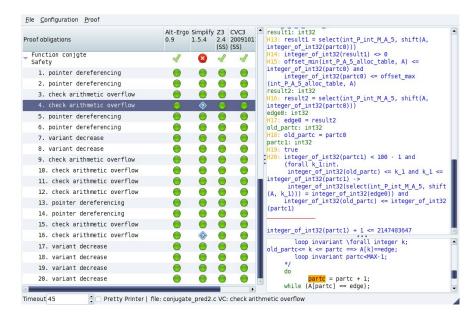


Fig. 3. Graphical Interface: Safety

Next, data types must be simplified. Even if Frama-C can cope with simple structures, it is better to have a first pass on them (unions suppression, typedef expansion and so on).

How to Make Good Annotations? As previously explained, ACLS is a language which is used to annotate C programs. Annotating an existing program consists in choosing properties (comportment, results,...) that the user wants to be "confirmed", such as preconditions, loop invariants, post conditions. In our case, for example, one of the most relevant properties we proved is that the result B is the conjugate of the partition A. This property is stated as a postcondition.

As usual, there are several ways to formalize annotations. Particularly when using external provers, a good method is to know how provers work. Here, we have to remember that the automatic provers are SMT solvers (see section 2.2).

As an example, we can give the definition of countIfSup. In a first formalization we wrote it as an "axiomatization". But due to another problem that we will describe in the next paragraph, we needed to make some proofs in Coq which used countIfSup. Then, to make it easier for Coq, we decided to try to define it inductively. Thanks to this other definition, some conditions were automatically proved by SMT solvers. This example shows how important formalization choices can be.

In the next paragraph, we will explain and illustrate how Coq allowed us to correct some errors in our annotations.

Why Coq? Once annotations are completed, the method consists in using automatic provers (using gWhy for example). As previously explained, if all proof obligations are proved by at least one prover, the work can be considered as finished. But, if one or more proof obligations is/are still unproved, several approaches are possible: the first one consists in verifying that annotations are "sufficient", that is to say a precondition or a loop invariant is not missing. Another approach, when the user suppose that his annotations are correct, is to use an external non automatic prover to try to prove proof obligations that have not been verified previously.

In our case, we used the interactive theorem prover Coq twice. The first time was because a postcondition had not been proved by SMT provers. When we began Coq proof, we discovered that the definition of countIfSup was incomplete: the second part of the "||" (logical or) was missing.

The second time we used Coq was to prove a loop invariant. Similarly, we detected another incompleteness in countIfSup definition (j < MAX) instead of $j \leq MAX$). Proof assistants are well adapted to detect this kind of problems. Indeed, building formal proofs manually, a user can easily see which hypotheses are necessary.

After having corrected and replaced the "axiomatization" of countIfSup by a predicate, all proof obligations have been proved by at least one automatic prover.

Note that the new definition allowed us to remove from the annotations one additional lemma which, at first, appeared necessary.

Other Vicissitudes. Among the main encountered difficulties, we can mention the confidence in the provers we used. In our case, one of the versions of CVC3 was faulty and proved all VC correct, even when they were false. For this reason we decided to consider that a proof obligation was proved when at least two automatic provers succeed on proving it. It is the case for all our obligations except one (VC # 23 is only proved by Simplify). The proof of VC # 23 is in progress using Coq.

5 Conclusion and Future Work

We have isolated and formally proved one of the key commands of the SCHUR software. This work reinforced us in the idea of formally proving chosen parts of software of the same kind, composed of 40,000 lines of undocumented code.

Thanks to this approach, we have focused on critical points (such as particular initializations of arrays and appropriate bounds) from the original code and by extension, we have understood the progression axis of the methodology. In particular, it is better to know how SMT automatic provers work to try to make a "good" annotation so that obligation proofs will be more easily proved by them. In the methodology, non automatic external provers like Coq may be used to refine annotations, and to prove obligations when no automatic provers succeed.

The conjugate function is a basic brick of combinatorics. This give us perspective to prove other functions. Therefore, as a future work, the second step is to prove algorithms relying on exhaustive enumeration algorithm, such as computation of Littlewood-Richardson coefficients, Koskas numbers, Koskas matrices, representation multiplicity in tensor product decompositions, etc.

The final objective will be to build proved libraries usable for scientific community.

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